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Abstract

A formal perturbation theory is developed for Hamilton operators with purely discrete or with mixed (discrete and continuous) spectra. Formulas for the resolvent operator are given which exhibits the singularities and the discontinuities of the matrix elements of the resolvent in the representation in which the unperturbed Hamiltonian is diagonal. These results are applied to obtain a solution of the time-dependent Schrödinger problem. Two kinds of asymptotic expansions of this solution are then given. One expansion is valid for large values of the time; the other is valid for values of the time sufficiently large and for a sufficiently weak perturbation.

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1. Introduction

The aim of this paper is to investigate the formal theory of processes like scattering of particles, or the capture and the emission of a particle by a system. We are concerned especially with the case when the energy of the incident particle is close to the energy with which the particle can be bound, so that resonance phenomena occur. The particle could be a photon and the system an atom, or we can deal with nuclear particles and nuclei. The mathematical situation in all these cases is characterized by an unperturbed Hamiltonian having a mixed spectrum partly continuous and partly discrete, where some of the discrete eigenvalues lie inside the continuous spectrum. The problem is to evaluate the effect of a perturbation on such an unperturbed system and to solve the corresponding time-dependent Schrödinger problem, giving also asymptotic formulas for large values of the time.

Problems of the kind treated here have been the object of investigations by several authors. Most treatments are only approximate to a certain order in the strength of the interaction (usually to second order). This approach is presented for example by Dirac [2] in his discussion of collision problems. However, the very formulation of the problem in these papers is such that it is not at all clear how one should proceed if one wants to calculate higher approximations. Our solution of the problem exhibits the perturbed resolvent operator in terms of a closed set of equations. From these equations an iteration procedure immediately follows, which allows calculation to any order of accuracy in the perturbation parameter. A perturbation theory for the resolvent which allows calculations to all orders has also been developed by Heitler and his collaborators (see [6] where other literature is quoted). Their work, however, does not take fully into account all the significant consequences due to the presence of a continuous spectrum. In addition there appear to be some difficulties with their use of the concept of the diagonal part of certain operators. In our treatment the use of this concept is completely avoided. Also, we give expressions for all the matrix elements of the resolvent including some omitted by Heitler.

Perturbations of continuous spectra have been studied by Friedrichs [3]. One of the results of Friedrichs' paper is to give a precise mathematical meaning to the kind of approximation involved in the formulas given by Weisskopf and Wigner [1] in their treatment of natural line breadth. In Section 6 we shall show that his result follows quite easily from the properties of the resolvent operator.

The proofs given in the present paper are not mathematically rigorous; rather we shall follow a kind of heuristic method. Thus, instead of stating conditions to be satisfied by the perturbation and then proving that certain consequences follow, we shall simply assume that the perturbation is such that the necessary operations can be performed. Further, we often present our material not by treating the most general case, but instead by treating in detail certain special cases where the important features are clearly exhibited.

We shall solve the problems mentioned above by reducing them to the problem of the construction of the resolvent operator for the perturbed Hamiltonian H. The resolvent operator is defined as the operator

$$G(\lambda) = (\lambda - H)^{-1} , \tag{1}$$

where λ is a complex parameter. It is well known that the spectral theory of the operator H can be based on the consideration of its resolvent*. Here we shall only justify in a heuristic fashion some properties of the resolvent; similarly, we only give a heuristic justification of the formula (3) below, which is used in later considerations.

Let us call P_m the projection operator corresponding to the discrete eigenvalue λ_m of H, and P_E the projection operator corresponding to the value E

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* The importance of the resolvent operator in the solution of problems of the kind considered here has been emphasized by Schönberg [4], [5]. In [4] one can also find several mathematical references.

of the continuous spectrum. We can then write

$$(2) \qquad G(\lambda) = \sum_m \frac{P_m}{\lambda - \lambda_m} + \int \frac{P_E}{\lambda - E}\, dE ,$$

the integral being extended to the continuous spectrum of H. It is evident from (2) that the matrix elements of $G(\lambda)$ between two normalized states are analytic functions of λ which exhibit polar singularities at the eigenvalues λ_m and a discontinuity across the continuous spectrum.

Analytic functions of the operator H can be constructed in terms of the resolvent by a formula which is the analog of Cauchy's formula for analytic functions of a complex variable. Indeed one can easily convince oneself, using (2), that

$$(3) \qquad f(H) = \frac{1}{2\pi i} \oint_C f(\lambda) G(\lambda)\, d\lambda .$$

Here the function $f(\lambda)$ must be regular in all points of the spectrum of H and the integral is extended to a closed curve C (consisting of one or more closed loops) such that all eigenvalues of H lie to the left of C and all singularities of $f(\lambda)$ lie to the right. Of course, if the spectrum of H extends to infinity in the λ-plane, then the curve C must also extend to infinity.

We shall apply formula (3) to the case $f(\lambda) = e^{-i\lambda t}$ which has no singularities in the whole λ-plane, so that one can choose any contour surrounding the spectrum of H. Formula (3)then gives the solution of the time-dependent Schrödinger problem.

From the above discussion we see that our first task is to construct the resolvent of the perturbed Hamiltonian H in terms of the unperturbed Hamiltonian and the perturbation. This is done in Sections 2 and 3 for a purely discrete spectrum of simple eigenvalues, and is generalized in Section 4 for the case of a mixed

(discrete and continuous) spectrum, which is more important for our purposes.

We then use our results to obtain the asymptotic formulas which give the solutions of the time-dependent Schrödinger problem for large values of the time (Sections 5 and 6).

2. Perturbation of discrete spectra

In this section we shall give the formal theory of perturbation for the resolvent operator in the case of purely discrete spectra. From this, formulas for the eigenvalues and the eigenstates will be derived.

We consider an unperturbed Hamiltonian H^o which we assume to have a purely discrete spectrum. The eigenvalues, denoted by E_r, will be assumed to be simple. The total Hamiltonian $H = H^o + V$ will also have a discrete spectrum with simple eigenvalues, provided the perturbation V satisfies some conditions which we shall not investigate here. We are interested in the matrix elements $\langle E_r | G(\lambda) | E_s \rangle = G_{rs}(\lambda)$ of the resolvant $G(\lambda) = (\lambda - H)^{-1}$ in the representation in which the unperturbed Hamiltonian is diagonal. These matrix elements, considered as functions of the complex parameter λ, have polar singularities in the eigenvalues of H. We consider that eigenvalue λ_n of H which tends to a particular eigenvalue E_n of E as the perturbation tends to zero. We would like our formulas for $G_{rs}(\lambda)$ to exhibit clearly the polar singularity for $\lambda = \lambda_n$.

To this purpose we introduce the operator $\Gamma(\lambda)$, which is defined in the H^o- representation by the equation

$$(4) \qquad \Gamma_{rs}(\lambda) = V_{rs} + \sum_{t \neq n} V_{rt} \frac{1}{\lambda - E_t} \Gamma_{ts}(\lambda) \ .$$

Clearly $\Gamma(\lambda)$ depends upon the value n of the index which is omitted in the sum

occurring in the right-hand side, but we shall not indicate this dependence explicitly, since we want to concentrate on a particular value of n. Since the polar singularity for $\lambda = E_n$ does not appear in the equation, Γ can be assumed to be regular* in a neighborhood of E_n. Actually we shall see in Section 3 that Γ is regular for $\lambda = \lambda_n$.

We can now give the formulas for the matrix elements $G_{rs}(\lambda)$ in terms of the matrix elements $\Gamma(\lambda)$. The proof of these formulas will be given later; in this section we shall state them and shall derive some consequences from them. For the diagonal element $r = s = n$ one has

$$G_{nn}(\lambda) = \frac{1}{\lambda - E_n - \Gamma_{nn}(\lambda)} \quad . \tag{5}$$

The other matrix elements are given by

$$G_{rn}(\lambda) = \frac{1}{\lambda - E_r} \Gamma_{rn}(\lambda) \frac{1}{\lambda - E_n - \Gamma_{nn}(\lambda)} \qquad (r \neq n) , \tag{6}$$

$$G_{ns}(\lambda) = \frac{1}{\lambda - E_n - \Gamma_{nn}(\lambda)} \Gamma_{ns} \frac{1}{\lambda - E_s} \qquad (s \neq n) , \tag{7}$$

and finally, for r and s both different from n,

$$G_{rs}(\lambda) = \frac{\delta_{rs}}{\lambda - E_r} + \frac{1}{\lambda - E_r} \left[\Gamma_{rs}(\lambda) + \frac{\Gamma_{rn}(\lambda)\, \Gamma_{ns}(\lambda)}{\lambda - E_n - \Gamma_{nn}(\lambda)} \right] \frac{1}{\lambda - E_s} \quad . \tag{8}$$

These formulas show that the polar singularity of $G_{rs}(\lambda)$ in the vicinity of $\lambda = E_n$

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* When we say that an operator is regular, we mean that its matrix elements in the H^o-representation are regular.

is given by that root of

$$\lambda = E_n + \Gamma_{nn}(\lambda) \tag{9}$$

which tends to E_n when the perturbation V is made to tend to zero. This root (which is a simple root, from our assumptions) gives the eigenvalue λ_n we were interested in. We expect it to be real; and this is indeed the case, as can be shown using the reality properties of $\Gamma_{nn}(\lambda)$.

Incidentally, one sees very easily by giving r and s the appropriate values that (5), (6) and (7) are contained in (8). Therefore (8) is valid in general, without restriction on r and s. However, if r or s or both equal n, the simplified forms (5), (6) and (7) are more useful, because they do not show the denominator $\lambda - E_n$ which actually does not correspond to a singularity.

To find the eigenvector $|\lambda_n\rangle$ of H corresponding to λ_n we need the corresponding projection operator

$$P = \frac{1}{2\pi i} \oint_{\lambda_n} G(\lambda)\, d\lambda \quad , \tag{10}$$

where the integral is over a closed curve encircling λ_n but excluding all other eigenvalues of H. (Formula (10) follows immediately from (2).) One obtains from our formulas for $G_{rs}(\lambda)$ the expressions

$$P_{nn} = \frac{1}{2\pi i} \oint_{\lambda_n} \frac{1}{\lambda - E_n - \Gamma_{nn}(\lambda)}\, d\lambda \quad , \tag{11}$$

$$P_{rn} = \frac{1}{\lambda_n - E_r} \Gamma_{rn}(\lambda_n)\, P_{nn} \qquad (r \neq n) \quad , \tag{12}$$

$$P_{ns} = P_{nn}\, \Gamma_{ns}(\lambda_n) \frac{1}{\lambda_n - E_s} \qquad (s \neq n) \quad , \tag{13}$$

(14) $$P_{rs} = \frac{1}{\lambda_n - E_r} \Gamma_{rn}(\lambda_n) \, P_{nn} \, \Gamma_{ns}(\lambda_n) \frac{1}{\lambda_n - E_s} \qquad (r,s \neq n) \; .$$

Obviously, application of P to the eigenvector $|E_n\rangle$ of H^o gives $|\lambda_n\rangle$, apart from an arbitrary normalization factor. To obtain comparatively simple formulas it is convenient to choose $|E_n\rangle$ to be normalized, $\langle E_n|E_n\rangle = 1$, but $|\lambda_n\rangle$ such that

(15) $$\langle E_n|\lambda_n\rangle = 1 \; .$$

This means that we take

(16) $$|\lambda_n\rangle = \frac{P|E_n\rangle}{\langle E_n|P|E_n\rangle} \; .$$

With this choice of normalization, it follows from (12) that

(17) $$\langle E_r|\lambda_n\rangle = \frac{1}{\lambda_n - E_r} \Gamma_{rn}(\lambda_n) \qquad (r \neq n) \; .$$

This, together with (15), gives the coefficient of the development of $|\lambda_n\rangle$ as a linear combination of the normalized eigenvectors of the unperturbed Hamiltonian.

The formulas given in this section can be used to set up an approximation scheme, when the perturbation V is sufficiently small. The question of the exact conditions under which this is possible will be investigated in a future report.

3. Perturbation of discrete spectra (continuation)

We shall now prove the formulas (5) to (8) for the resolvent. For concise notation it is suitable to write the equations of this section without reference to a particular representation.

We introduce the projection operator

$$P^o = |E_n\rangle\langle E_n| \tag{18}$$

which projects on the eigenvector of H^o corresponding to the eigenvalue E_n. The equation which defines $\Gamma(\lambda)$ can be written now as

$$\Gamma(\lambda) = V + V(1 - P^o)\, G^o(\lambda)\, \Gamma(\lambda) \quad , \tag{19}$$

where $G^o(\lambda) = (\lambda - H^o)^{-1}$ is the unperturbed resolvent.

It is useful to find different forms for the relation satisfied by Γ. We first note that

$$\begin{aligned} (1 - P^o)G^o\Gamma &= G(\lambda - H^o - V)(1 - P^o)G^o\,\Gamma \\ &= G\left[(1 - P^o)\Gamma - V(1 - P^o)G^o\Gamma\right] \\ &= G\left[(1 - P^o)\Gamma - \Gamma + V\right] = G\left[V - P^o\Gamma\right] \quad . \end{aligned} \tag{20}$$

Here we have used the obvious fact that P^o commutes with G^o, and the equation (19) satisfied by Γ. Substituting (20) into (19), we obtain

$$\Gamma = V + VG\left[V - P^o\Gamma\right] \quad . \tag{21}$$

Now we remember that, by the very definition of G,

$$GV = G(\lambda - H^o) - 1 \tag{22}$$

and

$$VG = (\lambda - H^o)\, G - 1 \quad . \tag{23}$$

We first substitute (22) into (21) and obtain

$$\Gamma = VG(\lambda - H^o - P^o\Gamma) \quad . \tag{24}$$

Then, making use of (23), we can write

$$\Gamma = (\lambda - H^o)G(\lambda - H^o - P^o\Gamma) - (\lambda - H^o - P^o\Gamma) \quad . \tag{25}$$

If we write (25) in the H^o- representation, it is seen to contain all the relations (5) to (8) which express the resolvent in terms of Γ. To see this more explicitly without use of a particular representation, we can multiply (25) to the left by P^oG^o, which gives

$$P^o = P^oG(\lambda - H^o - P^o\Gamma) \; . \tag{26}$$

This formula is clearly equivalent to (5) and (7).

Now we observe that although λ is a complex parameter, the operators G, G^o and Γ are functions of λ 'with Hermitian coefficients'. This means that, for instance,

$$\overline{\Gamma}(\lambda) = \Gamma(\bar{\lambda}) \quad . \tag{27}$$

Therefore if (26) holds then also

$$P^o = (\lambda - H^o - \Gamma P^o)\, GP^o \tag{28}$$

holds. To prove this, one need only take the Hermitian conjugate relation of (26), noting that $\bar{\lambda}$ is an arbitrary complex number, just as λ is. Of course the same observation applies to any of the other relations between operators we are dealing with.

Using (28), we can write (25) as

$$\Gamma = (\lambda - H^o)G(\lambda - H^o) - (\lambda - H^o) - \Gamma P^oGP^o\Gamma \quad , \tag{29}$$

which, when solved for G, gives

(30) $$G = G^o + G^o \left[\Gamma + \Gamma P^o G P^o \Gamma\right] G^o \quad .$$

Using (26), we find that this last formula becomes identical with the relation (8), which we wanted to prove.

Finally we want to give a relation for Γ which involves the resolvent G in a more symmetrical form than (21) and (24) do. We obtain it by substituting into (21) the relation

(31) $$\Gamma = (\lambda - H^o - \Gamma P^o)\, GV$$

which follows from (24). In this way we get

(32) $$\Gamma = V + V\left[G - GP^o(\lambda - H^o - \Gamma)P^o G\right] V \quad .$$

We can now give an argument to the effect that the operator $\Gamma(\lambda)$ is regular for $\lambda = \lambda_n$. Writing (32) in the H^o- representation, and taking into account (5), we obtain

(33) $$\Gamma_{rs} = V_{rs} + \sum_{t,\ell} V_{rt}\left[G_{t\ell} - \frac{G_{tn}G_{n\ell}}{G_{nn}}\right] V_{\ell s} \quad .$$

This formula gives Γ if G is known; it can be considered the inverse of (8). Now, as we are going to show immediately, the combination of matrix elements of the resolvent which appears in the square brackets in (33) is regular for $\lambda = \lambda_n$. Therefore, under certain assumptions on the matrix elements V_{rs}, the elements $\Gamma_{rs}(\lambda)$ are also regular for $\lambda = \lambda_n$.

To investigate the behavior of $G_{t\ell} - \dfrac{G_{tn}G_{n\ell}}{G_{nn}}$ at $\lambda = \lambda_n$, we first recall that

(34) $$G_{t\ell} = \sum_h \frac{\bar{c}_{ht} c_{h\ell}}{\lambda - \lambda_h} \quad ,$$

where $c_{h\ell} = \langle \lambda_h | E_\ell \rangle$ (here all the eigenvectors are taken to be normalized). Then we have

$$(35) \qquad \frac{G_{tn} G_{n\ell}}{G_{nn}} = \frac{\sum_{hk} \frac{\bar{c}_{ht} c_{hn}}{\lambda - \lambda_h} \frac{\bar{c}_{kn} c_{k\ell}}{\lambda - \lambda_k}}{\sum_r \frac{\bar{c}_{rn} c_{rn}}{\lambda - \lambda_r}} .$$

Since for a sufficiently weak perturbation we certainly have $\bar{c}_{nn} c_{nn} \neq 0$, we can say that the right-hand side of (35) has a simple pole for $\lambda = \lambda_n$, and that the coefficient is

$$(36) \qquad \frac{\bar{c}_{nt} c_{nn} \bar{c}_{nn} c_{n\ell}}{\bar{c}_{nn}\, c_{nn}} = \bar{c}_{nt}\, c_{n\ell} .$$

But this is the coefficient of $\frac{1}{\lambda - \lambda_n}$ in $G_{t\ell}$; we see now that the polar singularities of the terms occurring in (33) in square brackets cancel when one takes the difference.

4. Perturbation of mixed spectra

The work of the preceding sections can be generalized without much difficulty to the case of an unperturbed Hamiltonian which has a purely continuous spectrum or a mixed spectrum (discrete and continuous). In this section we shall treat this latter case, which is more comprehensive. Specifically, we consider an unperturbed Hamiltonian describing the system of a particle and a scatterer (cf. Dirac [2], Chapter 8), when there exist states in which the particle is bound to the scatterer. The unperturbed Hamiltonian will then have a continuous spectrum, corresponding to the situation in which the particle has a given momentum and the scatterer is in a given state, and in addition it will also have a discrete spectrum,

corresponding to the situation in which the particle is bound to the scatterer. These bound states will be assumed to be orthogonal to each other and to the eigenstates of the continuum, although this may only be approximately true for actual physical systems (see Dirac [2], 51). The energies of these bound states may lie outside the continuous spectrum, or may correspond to values of the continuous spectrum. In the latter case we say that the discrete eigenvalues are embedded in the continuous spectrum.

We now introduce a perturbation. The effect will be a change of the discrete states and their energies; the continuous spectrum will be assumed to remain the same and only the corresponding eigenfunctions will undergo a change. Formulas for the perturbed resolvent which exhibit the polar singularity corresponding to one particular discrete eigenvalue can easily be obtained by generalizing the formulas given in the preceding sections for the case of a purely discrete spectrum. All formulas which are written without reference to the H^o- representation can be taken over as they stand. The essential new feature occurring now is the discontinuity that G^o, and therefore Γ and G, exhibit as functions of λ across the continuous part of the spectrum. Let us consider for instance the resolvent $G(\lambda)$. For a specific value of the energy E of the continuous spectrum $G(\lambda)$ takes two different values according as one approaches the point E from the positive or the negative imaginary side.

An important consequence of this discontinuity is that one can try to continue analitically the matrix elements of the operators involved across the continuous spectrum into what we shall call the second sheet of the plane of the complex variable λ. We shall assume that this analytic continuation is actually possible to some extent. In a certain region of the complex λ-plane surrounding the continuous spectrum we then obtain two branches of the analytic function $G(\lambda)$; using conventional notation, we write $G^+(\lambda)$ for

that branch which goes into the resolvent $G(\lambda)$ of the first sheet on the positive imaginary side of the continuous spectrum and $G^{-}(\lambda)$ for the one which agrees with $G(\lambda)$ on the negative imaginary side of the continuous spectrum. The same notation will be used for Γ and G^{o}.

Turning now to the discrete eigenvalues, we see that a very special situation can occur if the eigenvalue E_n is embedded in the continuous spectrum. By application of formulas analogous to those developed for the case of discrete spectra, we would expect the discrete eigenvalue E_n to undergo a shift of position when the perturbation is switched on. If we consider E_n as a pole of $G^{o+}(\lambda)$, the perturbed position of the pole will be given by that root of the equation

$$(37) \qquad \lambda = E_n + \langle n | \Gamma^{+}(\lambda) | n \rangle$$

which tends to E_n when the perturbation tends to zero. It will be shown below that in general this root has a negative imaginary part. This means that the perturbed Hamiltonian does not have a discrete eigenvalue at all, although the matrix elements of the resolvant have a polar singularity below the real axis in the second sheet. The discrete eigenvalue has disappeared under the influence of the perturbation. This situation is rather typical for discrete eigenvalues embedded in the continuous spectrum (see Friedrichs [3]).

In the case just discussed the matrix elements of the perturbed resolvant are given by formulas quite analogous to (5), (6), (7) and (8). We write them here explicitly, since we are going to use them later. For simplicity we consider the case when there is only one simple discrete eigenvalue and this is embedded in the continuum. We denote by $|E\rangle$ the eigenvector of H^{o} corresponding to a value E of the continuous spectrum, without indicating explicitly the other variables which refer

to the direction of the motion of the particle and to the state of the scatterer. Thus when integrations or sums with respect to these variables occur (as for instance in formula (42) below) these operations will also not be explicitly indicated. Furthermore, we simply write $|n\rangle$ for the discrete eigenstate of unperturbed energy E_n. We then have

(38) $$\langle n|G|n\rangle = \frac{1}{\lambda - E_n - \langle n|\Gamma(\lambda)|n\rangle} ,$$

(39) $$\langle E|G|n\rangle = \frac{1}{\lambda - E} \langle E|\Gamma(\lambda)|n\rangle \frac{1}{\lambda - E_n - \langle n|\Gamma(\lambda)|n\rangle} ,$$

(40) $$\langle n|G|E\rangle = \frac{1}{\lambda - E_n - \langle n|\Gamma(\lambda)|n\rangle} \langle n|\Gamma(\lambda)|E\rangle \frac{1}{\lambda - E} ,$$

(41) $$\langle E|G|E'\rangle = \frac{\langle E|E'\rangle}{\lambda - E} + \frac{1}{\lambda - E}\left[\langle E|\Gamma|E'\rangle + \frac{\langle E|\Gamma|n\rangle\langle n|\Gamma|E\rangle}{\lambda - E_n - \langle n|\Gamma|n\rangle}\right]\frac{1}{\lambda - E'} .$$

We recall here also the definition of Γ, which, written explicity in the H^o- representation, now reads

(42) $$\Gamma(\lambda) = V + V\int \frac{|E\rangle\, dE\, \langle E|}{\lambda - E}\,\Gamma(\lambda) .$$

The integral is extended to the continuous spectrum of H^o, and, from our assumption that only one discrete eigenstate is present, it is seen to be equal to $G^o(\lambda)(1-P^o)$, where $P^o = |n\rangle\langle n|$.

Now we wish to investigate the reality properties of the operator $\Gamma(\lambda)$. Of course we assume that H^o and V are Hermitian operators.

We recall that by definition

(43) $$\Gamma(\lambda) = V + V(1 - P^o)G^o(\lambda)\Gamma(\lambda) .$$

From this we can prove

(44) $$\overline{\Gamma}(\lambda) = \Gamma(\bar{\lambda}) ,$$

i.e., Γ is a function of λ with Hermitian coefficients. Taking $\lambda = E$ to be real and outside of the continuous spectrum, one concludes that the operator $\Gamma(E)$ is Hermitian.

We know however, that in the case where H^o has a continuous spectrum and E lies in it, $\Gamma(E)$ has two different values $\Gamma^+(E)$ and $\Gamma^-(E)$ obtained by approaching the real axis from the positive or from the negative imaginary side respectively. In this case (44) can be used to show that

(45) $$\overline{\Gamma}^+(E) = \Gamma^-(E) .$$

To find out more, we use the equation

(46) $$\Gamma(\lambda) = V + \Gamma(\lambda)(1 - P^o)G^o(\lambda)V$$

which, in accordance with the observation following equation (28), is also satisfied by Γ. The expression

$$\left[1 + \Gamma(\lambda)(1 - P^o)G^o(\lambda)\right] V \left[1 + (1 - P^o)G^o(\lambda')\Gamma(\lambda')\right]$$

can be simplified by use of either (43) or (46). The equality relation of the two resulting expressions

$$\left[1 + \Gamma(\lambda)(1 - P^o)G^o(\lambda)\right]\Gamma(\lambda') = \Gamma(\lambda)\left[1 + (1 - P^o)G^o(\lambda')\Gamma(\lambda')\right]$$

can be written

(47) $$\Gamma(\lambda) - \Gamma(\lambda') = \Gamma(\lambda)(1 - P^o)\left[G^o(\lambda) - G^o(\lambda')\right]\Gamma(\lambda') .$$

If in this formula we take $\lambda = E + i\sigma$, $\lambda' = E - i\sigma$ and make use of (44),

we obtain

$$\Gamma(E + i\sigma) - \Gamma(E - i\sigma) = \Gamma(E + i\sigma) - \bar{\Gamma}(E + i\sigma)$$

$$= \Gamma(E + i\sigma)(1 - P^0)\left[G^0(E + i\sigma) - G^0(E - i\sigma)\right]\bar{\Gamma}(E + i\sigma) \quad .$$

Now we let σ tend to zero. Remembering that

$$(48) \qquad \lim_{\sigma \to 0} \left[G^0(E + i\sigma) - G^0(E - i\sigma)\right] = - 2\pi i\ \delta(E - H^0)$$

we have

$$(49) \qquad \frac{\Gamma^+(E) - \bar{\Gamma}^+(E)}{2i} = - \pi\ \Gamma^+(E)(1 - P^0)\delta(E - H^0)\bar{\Gamma}^+(E) \quad .$$

In words: the anti-Hermitian part of $\Gamma^+(E)$ is a negative definite operator (with E lying in the continuous spectrum). It follows in particular, since $\delta(E - H^0) = |E\rangle\langle E|$, that

$$(50) \qquad \mathrm{Im}\ \langle n|\Gamma^+(E)|n\rangle = - \pi \left| \langle n|\Gamma^+(E)|E\rangle \right|^2 \leq 0 \quad .$$

We shall assume now that $\langle n|\Gamma^+(E)|E\rangle \neq 0$ for all values E of the continuous spectrum. The imaginary part of $\langle n|\Gamma^+(E)|n\rangle$ is then negative for all those values. This means that the equation (37) cannot have a real root lying in the continuous spectrum. On the other hand, it cannot have a complex root in the first sheet of the λ-plane, since this would correspond to a complex eigenvalue for the Hermitian operator H. It follows then that if (37) has a root which approaches E_n when the perturbation tends to zero and if the perturbation is sufficiently small, this root must possess a negative imaginary part and lie in the second sheet of the λ-plane.

5. Asymptotic behavior of the solution of the time-dependent Schrödinger problem

We proceed now to investigate the asymptotic properties of the solution of the time-dependent Schrödinger equation for a perturbed Hamiltonian of the kind considered in Section 4. This problem can be reduced to the evaluation of the resolvent operator by means of the formula

$$e^{-iHt} = \frac{1}{2\pi i} \oint G(\lambda)\, e^{-i\lambda t}\, d\lambda \tag{51}$$

which we already discussed in Section 1. We remember that the contour of integration should encircle the whole spectrum of the Hamiltonian H. If the spectrum extends to infinity the contour will therefore also extend to infinity.

Specifically we are interested in the matrix elements of the operator e^{-iHt} in the representation in which H^0 is diagonal. These matrix elements have the physical meaning of transition amplitudes between eigenstates of the unperturbed Hamiltonian, from the time 0 to the time t. Since we have in formulas (38) to (41) the corresponding matrix elements of the resolvent G, our problem is solved by (51) in the form of a complex contour integral. This representation is very well suited for investigating the behavior of the matrix elements of e^{-iHt} for large t.

We shall give two kinds of asymptotic formulas. The first kind will be given in this section and is obtained by letting the time t tend to infinity while the other parameters remain fixed. The second asymptotic formula, which will be discussed later, gives the behavior of the matrix elements for times sufficiently large and for a sufficiently weak perturbation. In addition the matrix elements which refer to a transition to a state of the continuum are evaluated for unperturbed energies close to the energy of the discrete unperturbed eigenvalue. The

precise mathematical meaning of these statements will be given later.

We begin by writing explicitly the formulas which give the matrix elements we want to evaluate. The simplest case is that of the matrix element

$$(52) \qquad \left\langle n \middle| e^{-iHt} \middle| n \right\rangle = \frac{1}{2\pi i} \oint \frac{e^{-i\lambda t}}{\lambda - E_n - \left\langle n \middle| \Gamma(\lambda) \middle| n \right\rangle} \, d\lambda \, .$$

Since we want to investigate the behavior of the integral for large t, it is convenient to change the contour of integration so that λ has everywhere a negative imaginary part on it. This is possible only by moving the upper half of the contour through the continuous spectrum into the second sheet so that it lies below the real axis. We see in this way that $\left\langle n \middle| e^{-iHt} \middle| n \right\rangle$ tends to zero as $t \rightarrow \infty$. This result is rather obvious from a physical point of view.

We proceed now quite similarly for the other matrix elements of e^{-iHt}. We have

$$(53) \qquad \left\langle E \middle| e^{-iHt} \middle| n \right\rangle = \frac{1}{2\pi i} \oint \frac{e^{-i\lambda t}}{\lambda - E} \left\langle E \middle| \Gamma(\lambda) \middle| n \right\rangle \frac{1}{\lambda - E_n - \left\langle n \middle| \Gamma(\lambda) \middle| n \right\rangle} \, d\lambda \, .$$

Moving the contour as before, we cross this time a polar singularity for $\lambda = E$. Since the integral over the new contour vanishes asymptotically for large values of t, we can write

$$(54) \qquad \lim_{t \rightarrow \infty} e^{iEt} \left\langle E \middle| e^{-iHt} \middle| n \right\rangle = \left\langle E \middle| \Gamma^{+}(E) \middle| n \right\rangle \frac{1}{E - E_n - \left\langle n \middle| \Gamma^{+}(E) \middle| n \right\rangle} \, .$$

Notice that because of the way we moved the contour of integration the Γ^{+} branch of the function $\Gamma(\lambda)$ is the one that occurs in formula (54). We have obtained in this way the final value of the transition amplitude from the discrete eigenstate $|n\rangle$ into the eigenstate $|E\rangle$ of the continuum. Remembering that the denominator has a complex zero λ_n near to the value E_n of the energy, we can say

that the transition amplitude just mentioned must have a sharp maximum for E = real part of λ_n.

Finally we are interested in the matrix element

(55) $$\langle E|e^{-iHt}|E'\rangle = \langle E|E'\rangle e^{-iEt} + \frac{1}{2\pi i}\oint \frac{e^{-i\lambda t}}{\lambda - E}\langle E|R(\lambda)|E'\rangle \frac{1}{\lambda - E'}\, d\lambda ,$$

where we have set

(56) $$\langle E|R(\lambda)|E'\rangle = \langle E|\Gamma(\lambda)|E'\rangle + \frac{\langle E|\Gamma|n\rangle\langle n|\Gamma|E'\rangle}{\lambda - E_n - \langle n|\Gamma|n\rangle} \quad .$$

In the same way as before, we obtain asymptotically

(57) $$\langle E|e^{-iHt}|E'\rangle \sim \langle E|E'\rangle + e^{-iEt}\langle E|R^{+}(E)|E'\rangle \frac{1}{E - E'}$$

$$+ \frac{1}{E' - E}\langle E|R^{+}(E')|E'\rangle\, e^{-iE't} \quad .$$

Remembering now that

(58) $$\lim_{t\to\infty} \frac{e^{it(E-E')}}{E - E'} = i\pi\delta(E - E')$$

we finally have

(59) $$\lim_{t\to\infty} e^{iEt}\langle E|e^{-iHt}|E'\rangle = \langle E|E'\rangle + \left[\frac{1}{E-E'} - i\pi\delta(E-E')\right]\langle E|R^{+}(E)|E'\rangle \quad .$$

The procedure we have used to pass from (57) to (59) is familiar from the theory of scattering. Formula (56) shows that the matrix elements of R^+ exhibit a resonance for E = real part of λ_n. The physical interpretation of the results of this section is well known. The real part of λ_n gives the displaced position of the center of the line which corresponds to the unperturbed energy E_n, while the absolute value of the imaginary part of λ_n gives the width of the line.

6. Second asymptotic expansion

In the preceding section we have given expressions for various matrix elements in the limiting case $t = \infty$. Now we shall give different asymptotic expressions, which show, in some cases, how those limiting values are approached as t increases.

We shall treat here explicitly the case in which all assumptions of the previous section concerning the spectrum are satisfied, and in addition the perturbation V is such that the matrix element $\langle n|V|n\rangle$ as well as all elements $\langle E|V|E'\rangle$ vanish. This case has been treated by Friedrichs [3] and the refined asymptotic expansion mentioned above was first stated in a precise mathematical form in his paper. We shall show that it follows very easily from our formulas.

Owing to the particular properties of the perturbation V, the equation (42) for the operator $\Gamma(\lambda)$ can be solved immediately. At this point it is useful to write $V = \varepsilon\mathcal{V}$, where ε is a parameter measuring the strength of the perturbation. As one can see very easily, the matrix elements of Γ are then given by

(60) $$\langle E|\Gamma|n\rangle = \varepsilon\langle E|\mathcal{V}|n\rangle \quad ,$$

(61) $$\langle n|\Gamma|E\rangle = \varepsilon\langle n|\mathcal{V}|E\rangle \quad ,$$

(62) $$\langle E|\Gamma|E'\rangle = 0 \, ,$$

(63) $$\langle n|\Gamma|n\rangle = \varepsilon^2 \int \frac{\langle n|\mathcal{V}|E\rangle \, dE \, \langle E|\mathcal{V}|n\rangle}{\lambda - E} \quad ,$$

where we have made use of the conditions

(64) $$\langle E|\mathcal{V}|E'\rangle = 0$$

(65) $$\langle n|\mathcal{V}|n\rangle = 0 \quad .$$

These restrictions are not imposed on the perturbation only for the sake of simplicity. In actual physical problems, a correct choice of the unperturbed Hamiltonian will ensure that (65) is satisfied, i.e., that the first-order shift of the line vanishes. However, equation (64) will in general be replaced by the statement that the matrix element $\langle E|V|E'\rangle$ is of second order of smallness (proportional to ε^2) (cf. Dirac [2], § 51). It is easily seen that this less restrictive condition would suffice to obtain the results which we are interested in deriving.

Before we proceed further we must briefly consider the equation

$$\lambda = E_n + \langle n|\Gamma^+(\lambda)|n\rangle \tag{66}$$

which we have assumed to have a complex root λ_n below the real axis. Since the function $\langle n|\Gamma^+(\lambda)|n\rangle$ is assumed to be analytic in λ in a region containing the continuous spectrum, and is analytic in ε, we expect the root of (66) to be an analytic function of ε. As shown in the Appendix, this root can be constructed as a power series in ε, in terms of $\langle n|\Gamma^+(\lambda)|n\rangle$ and its derivatives with respect to λ, calculated for $\lambda = E_n$. These quantities can be expressed as improper integrals, extended to the continuous spectrum, involving the matrix elements of the perturbation. An approximation procedure for λ_n can be worked out in this way* which gives consistent results to all orders in ε. Here we need only the

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* It is usually stated that the power series expansion in ε for the shift of an eigenvalue embedded in the continuum breaks down, because if one tries to calculate the coefficients of terms containing powers of ε higher than the second, the results turn out to be infinite. However, we show in the Appendix that if this calculation is properly carried out one obtains a shift which is complex and analytic in ε.

rather trivial terms of second order, which are given for our special perturbation by

(67) $$\lambda_n = E_n + \varepsilon^2\alpha - i\varepsilon^2\beta + \left[\varepsilon^4\right]$$

with

(68) $$\alpha = \text{P.V.} \int \frac{\langle n|V|E\rangle dE \langle E|V|n\rangle}{E_n - E}$$

and

(69) $$\beta = \pi \langle n|V|E_n\rangle\langle E_n|V|n\rangle > 0 .$$

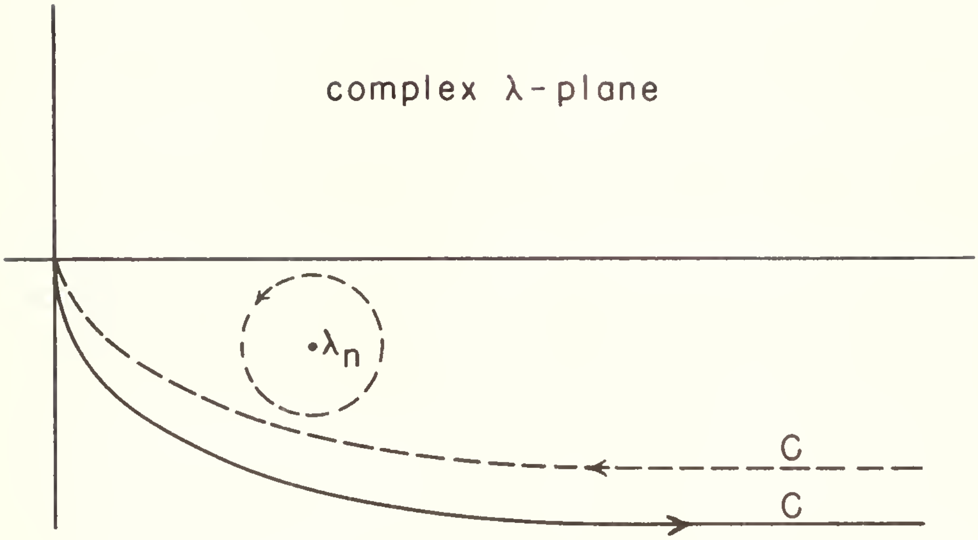
As indicated by the symbol P.V., the integral which gives α is to be evaluated as a principal value integral.

We can now proceed to the asymptotic evaluations. We begin again with the matrix element $\langle n|e^{-iHt}|n\rangle$, and wish to find its behavior as t tends to infinity while at the same time ε tends to zero in such a way that the product $\varepsilon^2 t$ remains finite. We can still use (52) and move the upper half of the contour below the real axis. However, since when $\varepsilon \to 0$, $\lambda_n \to E_n$, which is real, it is convenient now to move the contour across the polar singularity of the integrand for $\lambda = \lambda_n$. One obtains in this way

(70) $$\langle n|e^{-iHt}|n\rangle = e^{-i\lambda_n t}\, r_n + \frac{1}{2\pi i} \int_C$$

where the curve C lies as indicated in the figure and the residue in λ_n gives the factor

(71) $$r_n = \frac{1}{2\pi i} \oint_{\lambda_n} \frac{d\lambda}{\lambda - E_n - \langle n|\Gamma^+(\lambda)|n\rangle} .$$



The continuous spectrum, extending over the real axis from zero to infinity, is a line of discontinuity for the function $\langle n|G(\lambda)|n\rangle$. Dotted lines correspond to curves lying in the second sheet.

Now we note that when $\varepsilon \to 0$, then $\lambda_n \to E_n$ and $r_n \to \langle n|n\rangle = 1$. The contribution of the integral over C vanishes in the limit. As a consequence, with the above specified limiting process, we have

(72) $$\lim e^{iE_n t} \langle n|e^{-iHt}|n\rangle = e^{-it\varepsilon^2\alpha - t\varepsilon^2\beta}$$

or

(73) $$\langle n|e^{-iHt}|n\rangle \sim e^{-it(E_n + \varepsilon^2\alpha) - t\varepsilon^2\beta} .$$

This formula gives the exponential decay of the probability amplitude for the state $|n\rangle$ to remain unchanged. We want to emphasize that (73) follows from the particular way in which we assumed the perturbation to be weak. If one keeps the strength of the perturbation fixed, the decay of a state will not in general be exponential.

To obtain the asymptotic evaluation of the matrix element $\langle E|e^{-iHt}|n\rangle$ we shall perform a limiting process in which, when $t \to \infty$, $E \to E_n$ in such a way that $t(E - E_n)$ remains finite. In addition $\varepsilon \to 0$ as before, so that $t\varepsilon^2$ remains finite. The asymptotic formula which we obtain in this way (formula (76) below) will therefore give the matrix element for sufficiently large values of t, for a sufficiently weak perturbation and for values of the energy sufficiently near to E_n. We use (53) and move the contour as before. Then

$$\begin{aligned} \langle E|e^{-iHt}|n\rangle &= \langle E|\Gamma^+(E)|n\rangle \frac{e^{-iEt}}{E - E_n - \langle n|\Gamma^+(E)|n\rangle} \\ &+ \langle E|\Gamma^+(\lambda_n)|n\rangle \frac{e^{-i\lambda_n t}}{\lambda_n - E} r_n + \frac{1}{2\pi i}\oint_C \quad . \end{aligned} \tag{74}$$

With the specified limiting process we have

$$\lim t(E - \lambda_n) = t(E - E_n - \varepsilon^2\alpha + i\varepsilon^2\beta) = \lim t(E - E_n - \langle n|\Gamma^+(E)|n\rangle)$$

and

$$\lim t^{1/2} \langle E|\Gamma^+|n\rangle = t^{1/2}\varepsilon \langle E_n|V|n\rangle \quad .$$

Therefore we can state that

$$\lim t^{-1/2} e^{iEt} \langle E|e^{-iHt}|n\rangle = t^{1/2}\varepsilon\langle E_n|V|n\rangle \frac{1 - \exp\left[it(E - E_n - \varepsilon^2\alpha + i\varepsilon^2\beta)\right]}{t\left[E - E_n - \varepsilon^2\alpha + i\varepsilon^2\beta\right]} \tag{75}$$

or

$$\langle E|e^{-iHt}|n\rangle \sim \varepsilon\langle E_n|V|n\rangle \frac{\exp[-iEt] - \exp\left[-it(E_n + \varepsilon^2\alpha) - t\varepsilon^2\beta\right]}{E - E_n - \varepsilon^2\alpha + i\varepsilon^2\beta} \quad . \tag{76}$$

Finally, a similar method can be applied to the evaluation of $\langle E|e^{-iHt}|E'\rangle$. Here we must also let $E' \to E_n$ in such a way that $t(E' - E_n)$ remains finite. We do

not reproduce the complete calculation, which follows the same pattern as for the matrix elements evaluated above. The result is

$$\lim \frac{1}{t}\left[e^{iEt}\langle E|e^{-iHt}|E'\rangle - \langle E|E'\rangle\right] = t\varepsilon^2\langle E_n|\mathcal{V}|n\rangle\langle n|\mathcal{V}|E_n\rangle$$

$$(77)\quad \times\left[\frac{1}{t(E-E_n-\varepsilon^2\alpha+i\varepsilon^2\beta)t(E-E')} + \frac{\exp\left[it(E-E_n-\varepsilon^2\alpha+i\varepsilon^2\beta)\right]}{t(E-E_n-\varepsilon^2\alpha+i\varepsilon^2\beta)t(E'-E_n-\varepsilon^2\alpha+i\varepsilon^2\beta)} - \frac{\exp\left[it(E-E')\right]}{t(E'-E_n-\varepsilon^2\alpha+i\varepsilon^2\beta)t(E-E')}\right]$$

or

$$\langle E|e^{-iHt}|E'\rangle \sim \langle E|E'\rangle\, e^{-iEt} + \varepsilon^2\langle E_n|\mathcal{V}|n\rangle\langle n|\mathcal{V}|E_n\rangle$$

$$(78)\quad \times\left[\frac{\exp\left[-iEt\right]}{(E-E_n-\varepsilon^2\alpha+i\varepsilon^2\beta)(E-E')} + \frac{\exp\left[-it(E_n+\varepsilon^2\alpha)-t\varepsilon^2\beta\right]}{(E-E_n-\varepsilon^2\alpha+i\varepsilon^2\beta)(E'-E_n-\varepsilon^2\alpha+i\varepsilon^2\beta)} - \frac{\exp\left[-iE't\right]}{(E'-E_n-\varepsilon^2\alpha+i\varepsilon^2\beta)(E-E')}\right].$$

It is interesting to notice that if in the asymptotic formulas (76) and (78) we now let t tend to infinity, there result expressions similar to those given in (54) and (59) respectively, only with E substituted by E_n everywhere except in the first term of the resonance denominator. Also, if in (73) we let t tend to infinity, the expression vanishes, just as the exact matrix element given in (52) does.

Appendix. Solution of equation (66): $\lambda = E_n + \langle n | \Gamma^+(\lambda) | n \rangle$

In the case of a discrete eigenvalue embedded in the continuous spectrum, the perturbed resolvent has a pole for $\lambda = \lambda_n$, with λ_n a solution of (66). In this Appendix we shall investigate, somewhat more thoroughly than in the main text, the problem of solving (66) and in particular the construction of λ_n by an expansion in powers of the strength of the interaction. We shall concentrate on the simplified case treated in Section 6, so that (66) takes the form

$$\lambda = E_n + \varepsilon^2 \int \frac{|\langle n | \mathcal{V} | E \rangle|^2}{\lambda - E} \, dE \quad .$$

We are led in this way to the investigation of the solutions of an equation of the form

$$\text{(A.1)} \qquad \lambda = \lambda_0 + \alpha \int_a^b \frac{|f(E)|^2}{\lambda - E} \, dE \quad ,$$

where λ_0 lies inside the interval $[a,b]$. In actual physical problems the continuous spectrum extends from zero to infinity, but for reasons of simplicity we shall consider here the case of a finite interval. We also assume that the function $f(\zeta)$ is analytic and regular in a region R of the complex ζ-plane containing the interval $[a,b]$ in its interior. The function $\bar{f}(\zeta)$ is then an analytic function of $\bar{\zeta}$, let us call it $g(\bar{\zeta})$. Clearly $g(\zeta)$ is regular in a region S, which can be obtained from R by a reflection with respect to the real axis. The product

$$\text{(A.2)} \qquad f(\zeta)g(\zeta) = h(\zeta)$$

is regular in the intersection T of R and S, which is a region symmetric with respect to the real axis. For $\zeta = E$ real, we have

$$\text{(A.3)} \qquad h(E) = f(E)g(E) = f(E)\overline{f(E)} = |f(E)|^2 \quad .$$

We can write equation (A.1) in the form

$$\lambda = \lambda_o + \alpha \int_a^b \frac{h(E)}{\lambda - E}\, dE \tag{A.4}$$

and we know now that the function $h(\zeta)$ is regular in a region T of the complex ζ-plane which contains in its interior the interval $[a,b]$ of the real axis.

Consider now the function of λ

$$F(\lambda) = \int_a^b \frac{h(E)}{\lambda - E}\, dE \quad . \tag{A.5}$$

It is analytic in λ and its representation (A.5) shows that it is regular in the whole λ-plane with the possible exception of the interval $[a,b]$. Actually it is easily seen that this interval is a line of discontinuity, the jump across the real axis at the point E being given by

$$\lim_{\sigma \to 0} \left[F(E + i\sigma) - F(E - i\sigma) \right] = 2\pi i\, h(E) \quad . \tag{A.6}$$

As a consequence of the analyticity properties of $h(\zeta)$, one can continue $F(\lambda)$ across the discontinuity into a second sheet for the complex variable λ. For instance, if one approaches the discontinuity interval from the positive imaginary side, one can evaluate the integral along a curve C connecting a and b and lying below the real axis but inside the region T. In this way one sees that $F(\lambda)$ can be continued in the negative imaginary direction. The boundary of T poses a natural limitation to the continuation process. The endpoints a and b of the continuous spectrum appear as branch points for the function $F(\lambda)$. Following a notation already employed in the main text, we shall denote by $F^+(\lambda)$ the branch just constructed of the analytic function $F(\lambda)$, which is regular in a region containing

the open interval (a,b). Similarly, we would obtain $F^-(\lambda)$ approaching the line of discontinuity from the negative imaginary side.

Equation (A.4) can be written now more precisely as

$$\lambda = \lambda_o + \alpha F^+(\lambda), \tag{A.7}$$

where the function $F^+(\lambda)$ is regular in a region containing λ_o in its interior. It is clear that (A.7) admits a solution $\lambda = \lambda_\alpha$ which is analytic in α and approaches λ_o as α approaches zero. This solution can easily be given as a power series in α. Successive differentiation of (A.7) gives

$$\begin{aligned} \frac{d\lambda_\alpha}{d\alpha} &= F^+(\lambda_\alpha) + \alpha \frac{dF^+}{d\lambda_\alpha} \frac{d\lambda_\alpha}{d\alpha} , \\ \frac{d^2\lambda_\alpha}{d\alpha^2} &= 2 \frac{dF^+}{d\lambda_\alpha} \frac{d\lambda_\alpha}{d\alpha} + \alpha \frac{d^2F^+}{d\lambda_\alpha^2} \left(\frac{d\lambda_\alpha}{d\alpha}\right)^2 + \alpha \frac{dF^+}{d\lambda_\alpha} \frac{d^2\lambda_\alpha}{d\alpha} \end{aligned} \tag{A.8}$$

and so on. Setting $\alpha = 0$, we get

$$\begin{aligned} \lambda_\alpha\Big]_{\alpha = 0} &= \lambda_o \\ \frac{d\lambda_\alpha}{d\alpha}\Big]_{\alpha = 0} &= F^+(\lambda_o) \\ \frac{d^2\lambda_\alpha}{d\alpha^2}\Big]_{\alpha = 0} &= 2 \frac{dF^+}{d\lambda_\alpha} F^+(\lambda_\alpha)\Big]_{\lambda_\alpha = \lambda_o} \end{aligned} \tag{A.9}$$

and so on. Thus, to obtain the power series expansion for λ_α, one only needs to know the values of $F^+(\lambda)$ and its derivatives with respect to λ, calculated for $\lambda = \lambda_o$. Remembering (A.5) and (A.3), we can write these quantities as

$$(A.10) \qquad \left.\frac{d^n F^+(\lambda)}{d\lambda^n}\right]_{\lambda=\lambda_o} = \lim_{\sigma \to 0+} (-1)^n\, n! \int_a^b \frac{|f(E)|^2\, dE}{(\lambda_o + i\sigma - E)^{n+1}} \qquad (n = 0,1,2,\ldots) .$$

It is important to notice that the limits occurring in the right-hand side of (A.10) actually exist, although λ_o lies inside the interval of integration. Indeed, since $h(\zeta)$ is regular in the region T, one can integrate along the contour C mentioned above and obtain

$$(A.11) \qquad \lim_{\sigma \to 0+} \int_a^b \frac{|f(E)|^2\, dE}{(\lambda_o + i\sigma - E)^{n+1}} = \int_C \frac{h(\zeta)\, d\zeta}{(\lambda_o - \zeta)^{n+1}} .$$

Concerning reality properties, we notice that all quantities given in (A.10) for $n > 0$ are real. This one can see from the fact that the complex conjugate of $\left.\frac{d^n F^+}{d\lambda^n}\right]_{\lambda=\lambda_o}$ would be obtained by a formula similar to (A.10) only with σ tending to zero through negative values. In the analog of (A.11) one would then have an integral over a curve C' lying above the real axis. However, this curve can be moved to coincide with C, since the residue at the pole λ_o vanishes for $n > 0$. Hence $\left.\frac{d^n F^+}{d\lambda^n}\right]_{\lambda=\lambda_o}$ coincides with its complex conjugate. For $n = 0$, one has the familiar expression

$$(A.12) \qquad F^+(\lambda_o) = \text{P.V.} \int_a^b \frac{|f(E)|^2 dE}{\lambda_o - E} - i\pi |f(\lambda_o)|^2 ,$$

where the integral has to be evaluated as a principal value integral. In this case the negative imaginary part $-\pi|f(\lambda_o)|^2$ results.

It is clear from the above work that the case in which λ_o lies outside of the interval $[a,b]$ would lead to the same formulas (A.9) and (A.10) for the

coefficients of the power series expansion of λ_a. However, in this case one can evaluate the limits in (A.10) by just setting $\sigma = 0$ in the integrand. The resulting formulas are then identical with standard perturbation theory. This shows that the case treated here of a discrete eigenvalue embedded in the continuous spectrum can be considered as solved essentially by standard perturbation theory if one adds the provision that the singular integrals occurring must be evaluated by the limiting process specified in (A.10). This limiting process extracts, so to speak, the finite part of integrals of the kind

$$\int_a^b \frac{|f(E)|^2 dE}{(\lambda_o - A)^{n+1}} \qquad (n > 0)$$

with λ_o contained inside the interval $[a,b]$. It would be easy to see that the present definition of the finite part of an integral is identical with the definition given by Hadamard [7] and widely used in the mathematical literature.

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